D-3 3

Mr Bowen
Interplane
Lanes
Alex

LAMS-2365

LOS ALAMOS SCIENTIFIC LABORATORY

OF THE UNIVERSITY OF CALIFORNIA ○ LOS ALAMOS NEW MEXICO

WAT: A NUMERICAL METHOD FOR TWO-DIMENSIONAL UNSTEADY FLUID FLOW

Index

(1) Hydrodynamics, Machine Methods for two-dimensional Problems

(2) Fluid Flow, Machine computations in two dimensions

LEGAL NOTICE

Printed in USA. Price $ .50. Available from the

Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.

LAMS-2365
PHYSICS AND MATHEMATICS
(TID-4500, 15th Ed.)

LOS ALAMOS SCIENTIFIC LABORATORY
OF THE UNIVERSITY OF CALIFORNIA LOS ALAMOS NEW MEXICO

REPORT WRITTEN: September 20, 1960

REPORT DISTRIBUTED: November 11, 1960

WAT: A NUMERICAL METHOD FOR TWO-DIMENSIONAL UNSTEADY FLUID FLOW

by

Walter B. Goad

Contract W-7405-ENG. 36 with the U. S. Atomic Energy Commission

ABSTRACT

A method is described in which difference equations are derived by application of the principle of virtual work to a particular fluid model. Some other innovations involve the viscous pressure, different time intervals for different points, and a method of handling the collision of free interfaces.

These notes describe several innovations in Lagrangian, time-dependent, two-dimensional hydrodynamics. These are incorporated in a code called WAT now in use on the LASL IBM Model 704 computers. When applied to problems that involve only one-dimensional motion it appears to be as accurate as one-dimensional treatments with comparable mesh size. In several two-dimensional problems it has given reasonable results.

I. The Fluid Model -- Differential and Difference Equations

We partition the fluid into a number of discrete zones, adopt a specific physical model of the partitioned fluid, and use D'Alembert's principle to obtain exact equations of motion for the model. These are differential equations in time, and we difference them in a straightforward way.

The fluid is divided into cells of quadrilinear cross section, as in Figure 1. We will take all inertia to be concentrated on point particles at the cell vertices; the material within each cell exerts

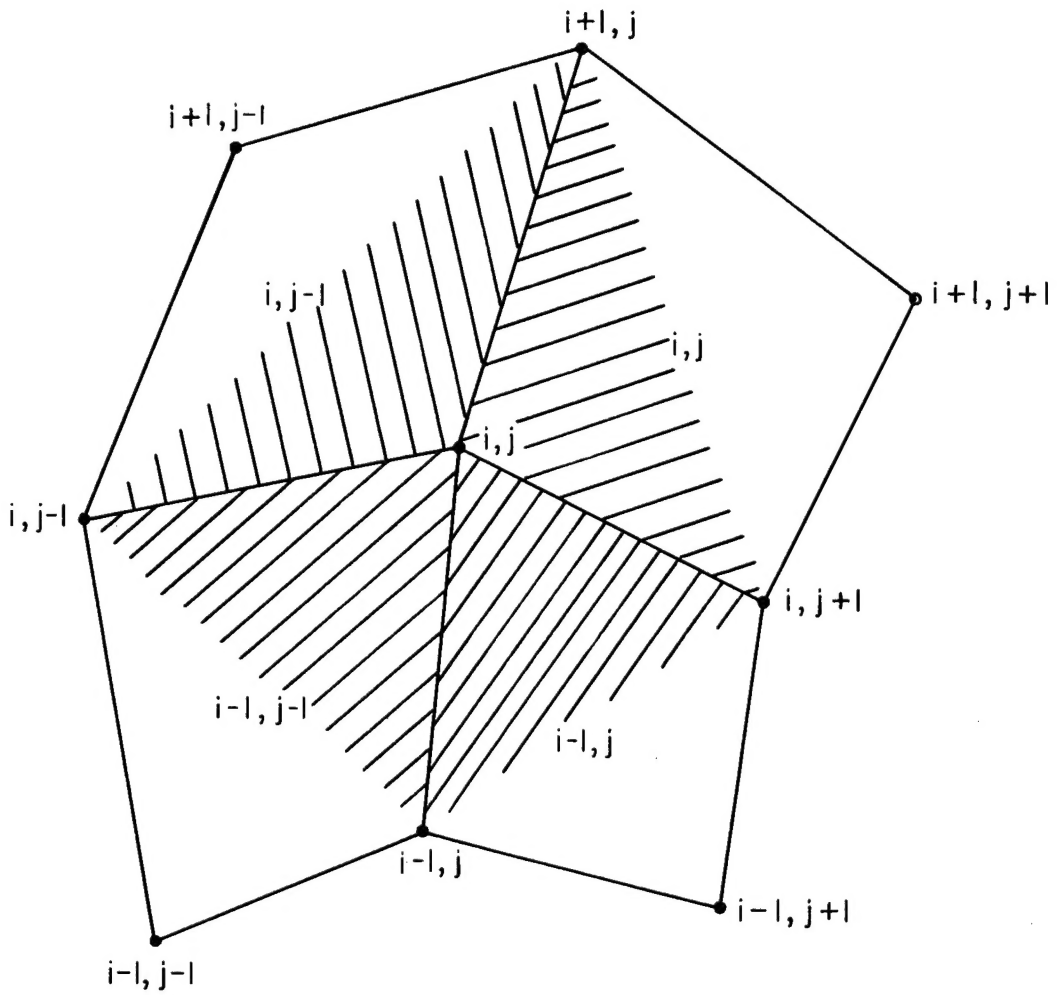

Figure 1

pressure determined through an equation of state by its internal energy E and volume V.

Suppose point (i,j) is displaced infinitesimally by $\delta\underline{s}$. Work is done on the surrounding four cells and the system's energy is modified by δE.

$$\delta E = p_{ij}\,\delta\underline{s}\cdot\underline{\nabla V}_{ij} + p_{ij-1}\delta\underline{s}\cdot\underline{\nabla V}_{ij-1} + p_{i-1,j-1}\delta\underline{s}\cdot\underline{\nabla V}_{i-1,j-1} + p_{i-1,j}\delta\underline{s}\cdot\underline{\nabla V}_{i-1j}. \tag{1}$$

According to a general principle of mechanics (D'Alembert's principle) a force $\underline{F}$ acts on the particle (i,j)

$$\delta E = \underline{F}_{ij}\cdot\delta\underline{s}$$

or

$$\underline{F}_{ij} = p_{ij}\underline{\nabla V}_{ij} + p_{i,j-1}\underline{\nabla V}_{i,j-1} + p_{i-1,j-1}\underline{\nabla V}_{i-1,j-1} + p_{i-1,j}\underline{\nabla V}_{i-1,j}. \tag{1'}$$

The equation of motion of point (i,j) is then

$$\ddot{\underline{r}}_{ij} = \frac{\underline{F}_{ij}}{M_{ij}} \tag{2}$$

which may be differenced in time

$$\frac{\underline{r}_{ij}^{t+\Delta t} - 2\underline{r}_{ij}^{t} + \underline{r}_{ij}^{t-\Delta t}}{(\Delta t)^2} = \frac{\underline{F}_{ij}^{t}}{M_{ij}}. \tag{3}$$

In addition we need to keep account of the internal energy per unit mass through

$$d\epsilon_{ij} = \frac{p_{ij} dV_{ij}}{(\rho_o V_o)} \tag{4}$$

where $(\rho_o V_o)$ is the mass of fluid in the cell.

We take the mass M_{ij} of the particle at vertex (i,j) to be half the mass of the shaded regions in Figure 1.

The difference equations are written in full in the appendix for cylindrical (r,z) coordinates. It is a straightforward task to compute them for other coordinate systems. In cartesian (x,y) coordinates they reduce to Kolsky's equations[2] only for the case that the mesh is exactly rectangular.

Kolsky's equations are obtained by regarding the vertices as representative points fixed in a continuous fluid. A pressure gradient at the vertex is estimated and used to compute an acceleration. This can be done in many ways, and the present method can be regarded as just another, different, way of doing this. However, I would suggest that in a highly distorted mesh, where it is difficult to define a sensible

pressure gradient, the present method still makes physical sense -- the force on each particle is determined by the reaction of the mesh to its displacement.

II. Artificial Viscosity

To spread shock fronts over several zones, we introduce an artificial viscous pressure q, following Richtmyer and von Neumann[1]. A somewhat detailed interpretation of the viscous pressure's role is useful in finding a form appropriate to two dimensions. For example, our experience is that the isotropic form, q proportional to $(\frac{dV}{dt})^2$, is not adequate in a mesh far from square, where shocks coming from different directions see cells of quite different thickness.

In one dimension, Richtmyer and von Neumann's form for q can be written

$$q = a\rho(\Delta u)^2 \tag{5}$$

where ρ is the density in the cell, a is a dimensionless constant of the order of unity, and Δu is the velocity of approach of the two boundaries of the cell.

If Δu is a good deal smaller than sound velocity in the cell, no discontinuous behavior is expected and numerical integration should proceed smoothly. Addition of q to the pressure can be regarded as an

expedient to increase the sound velocity in the cell so that this condition is always met.

To see this, let the equation of state of the fluid be represented by a γ law,

$$p = (\gamma-1)\epsilon\rho$$

and we have the energy equation

$$d\epsilon = (p+q)\frac{d\rho}{\rho^2}.$$

The sound velocity is

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s = \left(\frac{\partial p}{\partial \rho}\right)_\epsilon + \left(\frac{\partial p}{\partial \epsilon}\right)_\rho \left(\frac{\partial \epsilon}{\partial \rho}\right)$$

$$= \frac{\gamma p}{\rho} + (\gamma-1)\frac{q}{\rho}$$

which can be written, using Eq. (5)

$$c^2 = c_o^2 + a(\gamma-1)(\Delta u)^2 \qquad (6)$$

where c_o is the sound velocity with $q=0$.

So, one sees, the effect of q is to add $(\Delta u)^2$ multiplied by a factor of the order of 1 to the square of the physical sound velocity,

and this will insure that two boundaries of a cell never approach each other rapidly compared with the effective sound velocity in the cell.

Following this interpretation, we have made q depend on the largest of the (6) velocities of approach of pairs of vertices of each cell, i.e.,

$$q = a\frac{(\rho_o V_o)}{V}\left[\frac{(\underline{\Delta u}\cdot\underline{r})^2}{r^2}\right]_{\text{max. of 6 pairs}} \qquad \text{some } \underline{\Delta u}\cdot\underline{r} < 0$$
$$= 0 \qquad \text{every } \underline{\Delta u}\cdot\underline{r} > 0 \tag{7}$$

where $\underline{\Delta u}$ and $\underline{r}$ represent the relative coordinate and velocity of a pair of vertices.

III. Stability

A few experiments with simple stability criteria using the sound transit time through an average, or alternatively, the smallest, dimension of a cell have convinced me of the value of a more accurate, if more complicated criterion. When the mesh became distorted, only a criterion using the smallest distance seemed adequate, and this wasted a great deal of computation by nearly always demanding too short an interval -- in the limit when two points coalesce, for example, a zero interval is demanded.

We obtain a more accurate criterion by, as usual, linearizing the equations of motion about an average motion, following von Neumann and Richtmyer[1]. Let δz_{ij}, δr_{ij} denote a (small) departure from the exact solution of the difference equation (3). The pressure in each cell will

change to first order in δz, δr, by

$$\delta p = \frac{\rho^2}{\rho_o V_o} c^2 \sum_{\substack{\text{all} \\ \text{vertices}}} \left[\frac{\partial V}{\partial z} \delta z + \frac{\partial V}{\partial r} \delta r \right] \tag{8}$$

where c is the sound velocity, $c^2 = \frac{\partial p}{\partial \rho}$, and the sum expresses the total change in V due to displacements at all four of its vertices. For the moment, we neglect the dependence of q, the viscous pressure, on the δ's. Then we obtain equations of motion for the δ's,

$$\begin{aligned} \frac{\delta z_{ij}^{t+\Delta t} - 2\delta z_{ij}^{t} + \delta z_{ij}^{t-\Delta t}}{\Delta t^2} = \frac{1}{M_{ij}} \left(\frac{\rho^2}{\rho_o V_o} c^2\right)_{ij} \left(\frac{\partial V_{ij}}{\partial z_{ij}}\right) \Bigg\{ & \frac{\partial V_{ij}}{\partial z_{ij}} \delta z_{ij} \\ & + \frac{\partial V_{ij}}{\partial r_{ij}} \delta r_{ij} + \frac{\partial V_{ij}}{\partial z_{i,j+1}} \delta z_{i,j+1} + \frac{\partial V_{ij}}{\partial r_{i,j+1}} \delta r_{i,j+1} \\ & + \frac{\partial V_{ij}}{\partial z_{i+1,j+1}} \delta z_{i+1,j+1} + \frac{\partial V_{ij}}{\partial r_{i+1,j+1}} \delta r_{i+1,j+1} + \frac{\partial V_{ij}}{\partial z_{i+1,j}} \delta z_{i+1,j} \\ & + \frac{\partial V_{ij}}{\partial r_{i+1,j}} \delta r_{i+1,j} \Bigg\} + \text{similar terms for neighboring cells} \\ & (i-1,j);\ (i-1,j-1);\ (i,j-1). \end{aligned} \tag{9}$$

There is a similar equation for $\delta \ddot{r}$. In a compressed notation for the right hand side,

$$\frac{\delta z_{ij}^{t+\Delta t} - 2\delta z^{t} + \delta z^{t-\Delta t}}{(\Delta t)^2} = D\delta_z^t. \tag{9'}$$

An accurate stability limit would be obtained by finding the largest eigenvalue of the (linear) operator D

$$D\delta z_{ij} = \omega_{max}^2 \delta z.$$

The solutions of difference equation (9) change character, from oscillatory (neutrally stable) to exponentially growing (unstable) as Δt is increased beyond Δt_{max},

$$(\Delta t_{max})^2 = \frac{4}{\omega_{max}^2}. \tag{10}$$

We construct a local stability limit for each point by replacing all of the factors $\frac{\partial V}{\partial z}\rho^2c^2$, $\frac{\partial V}{\partial r}\rho^2c^2$ by the largest of them.

We also use the larger of the two factors $\frac{\partial V_{ij}}{\partial z_{ij}}$, $\frac{\partial V_{ij}}{\partial r_{ij}}$. The largest eigenvalue will then occur for that mode in which all terms in the approximate D are in phase, and we construct a local Δt_{max} from an ω_{ij}^2 defined by

$$\omega_{ij}^2 = \frac{32}{M_{ij}} \left[\text{larger of} \left\{ \left| \frac{\partial V_{ij}}{\partial z_{ij}} \right| \right\} \right] \left\{ \begin{matrix} \text{largest} \\ \text{at any} \\ \text{vertex} \end{matrix} \left| \frac{\partial V}{\partial z} \right| \frac{\rho^2 c^2}{\rho_o V_o} \right\} = 4b_{ij}. \tag{11}$$

Another source of instability is the viscous pressure q, which depends on a relative velocity, Eq. (7). To first order in the perturbation a term will be added to the right hand side of Eq. (9) for each cell having (i,j) as a vertex. The one added to the terms written out in Eq. (9) is

$$\frac{1}{M_{ij}} \frac{\partial V_{ij}}{\partial z_{ij}} \frac{a(\rho_o V_o)_{ij}}{V_{ij}} \left[2|\Delta u|_z \, \Delta\left(\frac{\delta z^t - \delta z^{t-\Delta t}}{\Delta t}\right) + 2|\Delta u|_r \frac{\Delta(\delta r^t - \delta r^{t-\Delta t})}{\Delta t} \right].$$

As in Section II, Δ identifies the largest rate of approach of any pair of points around the cell. Again, we let all coefficients of the δ's take on the value of the largest one, and assume the mode that makes all of them add. The result is that we add to ω_{ij}^2, Eq. (11):

$$\frac{4b_{ij}^q}{\Delta t} = \frac{a}{M_{ij}} \frac{32}{\Delta t} \left[\text{larger of} \left\{ \left| \frac{\partial V_{ij}}{\partial z_{ij}} \right| \right\} \left[\begin{array}{l} \text{largest value} \\ \text{among the cells} \\ \text{of which } (i,j) \\ \text{is a vertex} \end{array} \right\} \left\{ \frac{\rho_o V_o}{V} |\Delta u| \right\} \right]. \quad (12)$$

And finally, Δt_{max} is determined for each point by

$$(\Delta t)^2 \, b_{ij}^o + \Delta t b_{ij}^q < 1. \quad (13)$$

IV. Use of Many Time Intervals

In many problems, a large reduction in computation can be realized

by moving each point with the time interval demanded for its stability. In this section the scheme used in WAT to do this is outlined.

Up to sixteen different time intervals are defined, each a factor two smaller than its predecessor. Each point's acceleration is then advanced with the largest interval that meets its stability criterion; its acceleration is taken constant over its interval, but its position is advanced as needed to advance the pressure in cells that touch a point being advanced with a smaller time interval. The velocity is always advanced to the center of the interval through which the position is to be advanced; positions are then always accurate to order $(\Delta t)^3$. A table (t^c_{ij}) is kept current of the time to which each position has been advanced, and another (t^v_{ij}) of the state of the velocities. In Figure 2 an outline flow chart of the calculation is shown. The time intervals are Δt_ω, $\omega = 0,1,2,\cdots,\omega_{max}$; Δt_o is the largest interval. F_ω and F^p_{ij} are flags (up or down) that tell, respectively whether a given interval has just been processed, and whether a given cell's pressure has been brought up to the current time. A table is available of the i,j coordinates of all points to be moved with a given interval Δt_ω.

V. Collision of Free Surfaces

WAT is provided with a routine for handling the collision of two free surfaces. In figure 3 a typical situation is depicted, where the points and cells have been numbered one dimensionally.

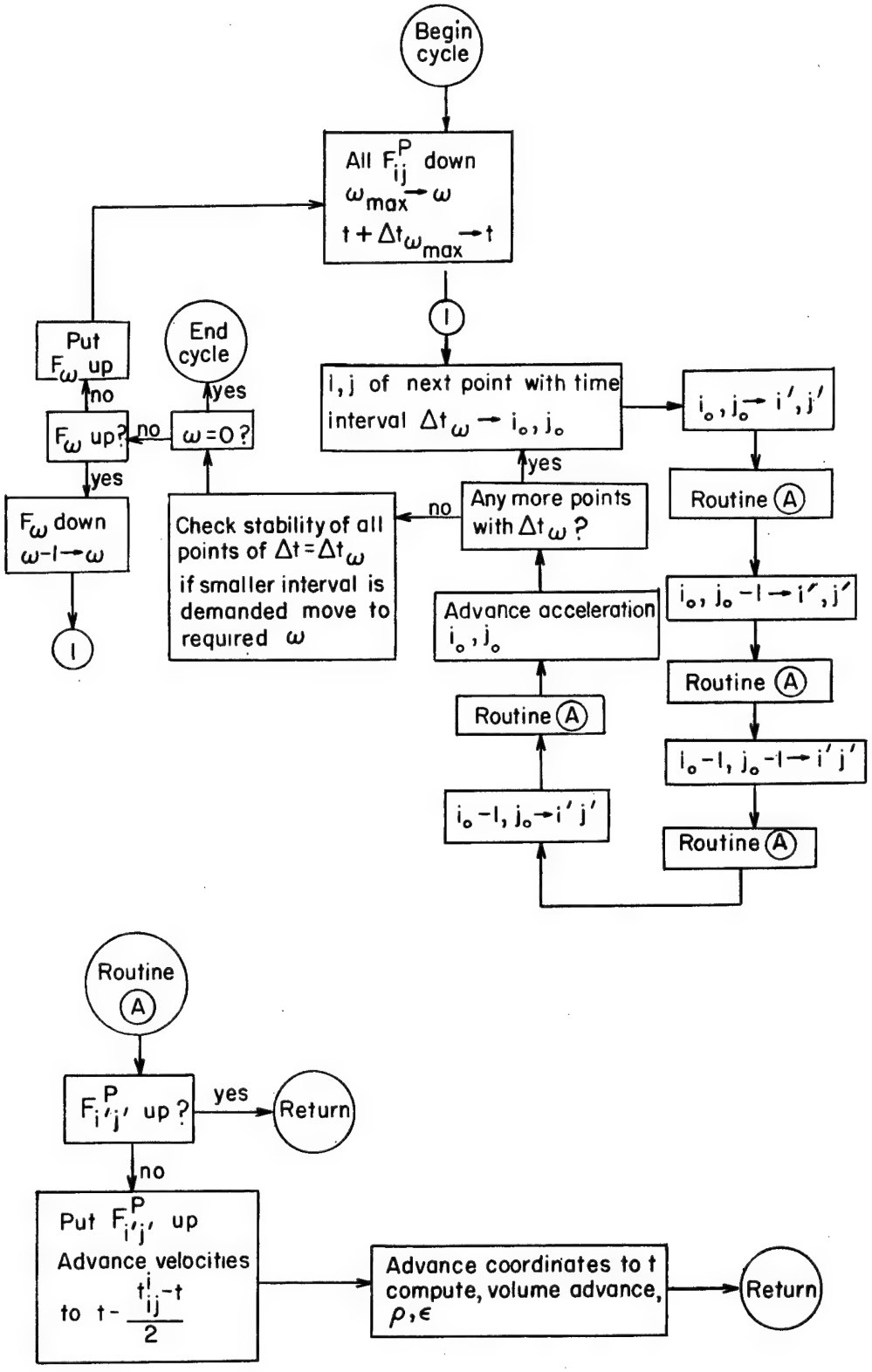
Begin cycle
All F^P_{ij} down
$\omega_{max} \rightarrow \omega$
$t + \Delta t_{\omega_{max}} \rightarrow t$
1
i, j of next point with time interval $\Delta t_\omega \rightarrow i_o, j_o$
$i_o, j_o \rightarrow i', j'$
Routine A
$i_o, j_o - 1 \rightarrow i', j'$
Routine A
$i_o - 1, j_o - 1 \rightarrow i' j'$
Routine A
$i_o - 1, j_o \rightarrow i' j'$
Routine A
Advance acceleration i_o, j_o
Any more points with Δt_ω ?
yes
no
Check stability of all points of $\Delta t = \Delta t_\omega$ if smaller interval is demanded move to required ω
$\omega = 0$?
yes
no
End cycle
F_ω up?
yes
no
F_ω down $\omega - 1 \rightarrow \omega$
Put F_ω up
1
Routine A
$F^P_{i'j'}$ up ?
yes
Return
no
Put $F^P_{i'j'}$ up
Advance velocities to $t - \frac{t^i_{ij} - t}{2}$
Advance coordinates to t compute, volume advance, ρ, ϵ
Return

Figure 2

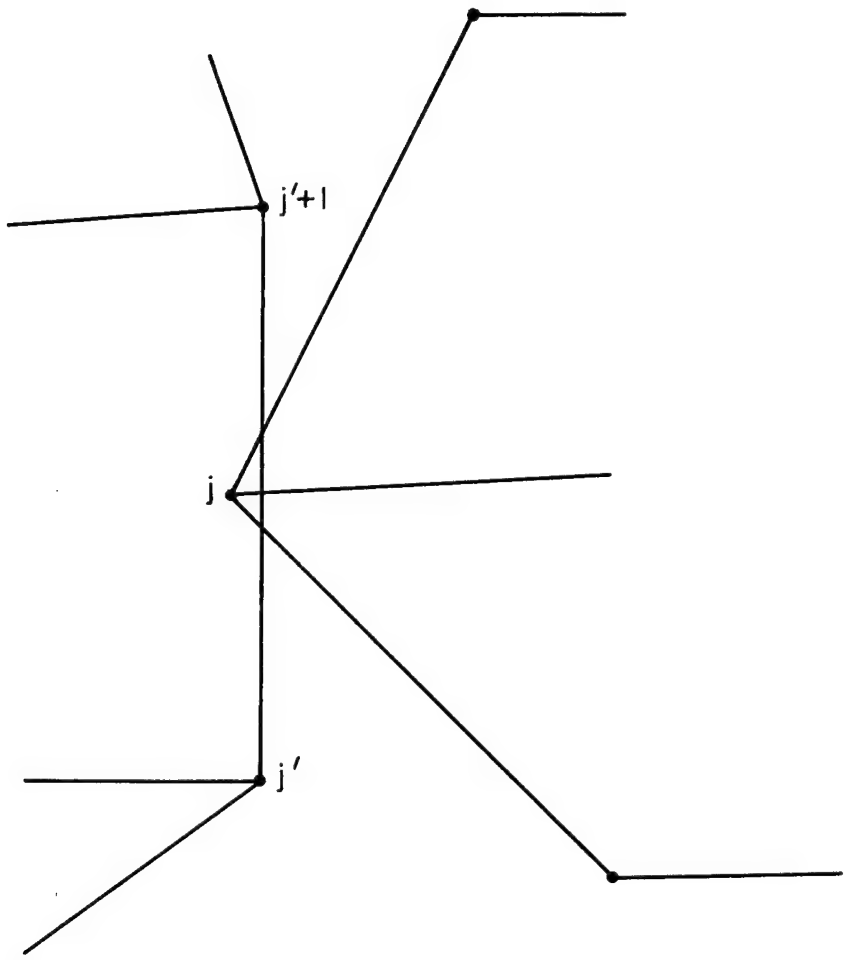

Figure 3

The first problem is to compute the time at which a point on one free surface crosses the other, as point j' has done. We make use of the sense of a point with respect to each line segment defining the surface that it may cross; it defines a point as being "inside" or "outside" of the region bounded by the line. The sense of point j with respect to the line through j', j'+1 is the sign of the expression

$$(z_j - z_{j'})(r_{j'+1} - r_{j'}) - (r_j - r_{j'})(z_{j'+1} - z_{j'}).$$

A point has not crossed a given segment unless its coordinates lie between those of the end points of the segment, within a tolerance given by the travel of the point during a time cycle, and unless its sense with respect to the segment has changed. When both of these conditions are fulfilled, we compute the time and coordinate of the intersection of the path of the particle with the segment. In general, one gets two solutions for each segment, and further, the above conditions may have been met for more than one segment, so the intersection is rejected unless the time of intersection is less than Δt, and unless the sense of the path -- from "outside to inside" -- is correct at the intersection.

In general it is necessary, for each point j, to examine every segment j', j'+1 of the opposing interface. The labor is reduced in WAT by first locating all of the points in a coarse Eulerian mesh. Then only if two points, not neighbors, fall within the same or neighboring cells does the code look for intersections. Possible crossings by each point

of every segment connected to one of the points are examined.

When a valid intersection is found, the three particles involved -- the intersecting one and the two that define the line segment -- are taken to collide inelastically. That is, the center of mass velocity is given to each of them, and the relative kinetic energy is distributed as internal energy among the participating cells.*

From then on, point j is attached to the interface of cell j'; that is, the volume of cell j' is computed using the segments j',j and j,j'+1 as its boundary, and the equation of motion of point j has a term

$$p_{j'} \underline{\nabla} V_{j'}$$

added to the force. It is necessary to maintain two tables: for each particle j, the cell to which it is attached, if any; for each cell j', the foreign point or points that are along its inner boundary, if any.

*Other models for the inelastic collision were tried, but this one led to the smoothest subsequent motion of the collision interface.

REFERENCES

1. J. von Neumann and R. D. Richtmyer, J. Appl. Phys. 21, 232 (1950)

2. H. Kolsky, LA-1867, April 1955

ACKNOWLEDGMENT

It is a pleasure to thank Chester Kazek, Ralph Anderson, and Jessie Rudnick for help in the programming of WAT.

APPENDIX

Difference Equations in Cylindrical Coordinates

The system is assumed rotationally symmetric about the r=0 axis. Indexing is as in Figure 1.

volume

$$V_{ij} = \frac{\pi}{3}(r_{ij}+r_{ij+1}+r_{i+j}) \left[(z_{ij+1}-z_{ij})(r_{i+1j}-r_{ij})\right.$$

$$\left. - (z_{i+1,j}-z_{ij})(r_{i,j+1}-r_{ij})\right]$$

$$+ \frac{\pi}{3}(r_{i+1j+1}+r_{i+1j}+r_{ij+1}) \left[(z_{i+1j}-z_{i+1j+1})(r_{ij+1}-r_{i+1j+1})\right.$$

$$\left. - (z_{ij+1}-z_{i+1j+1})(r_{i+1j}-r_{i+1j+1})\right]$$

acceleration

$$\frac{3}{\pi} M_{ij} \frac{(r_{ij}^{n+1} - 2r_{ij}^{n} + r_{ij}^{n-1})}{\Delta t^2} = p_{i-1,j} \begin{bmatrix} (r_{ij}+r_{i-1,j}+r_{i,j+1})(z_{i,j+1}-z_{i-1,j}) \\ + (z_{i-1,j}-z_{ij})(r_{i,j+1}-r_{ij}) \\ - (z_{i,j+1}-z_{ij})(r_{i-1,j}-r_{ij}) \end{bmatrix}$$

$$+ p_{ij} \begin{bmatrix} (r_{ij}+r_{i,j+1}+r_{i+1,j})(z_{i+1,j}-z_{i,j+1}) \\ + (z_{i,j+1}-z_{ij})(r_{i+1,j}-r_{ij}) \\ - (z_{i+1,j}-z_{ij})(r_{i,j+1}-r_{ij}) \end{bmatrix}$$

$$+ p_{i,j-1} \begin{bmatrix} (r_{ij}+r_{i+1,j}+r_{i,j-1})(z_{i,j-1}-z_{i+1,j}) \\ + (z_{i+1,j}-z_{ij})(r_{i,j-1}-r_{ij}) \\ - (z_{i,j-1}-z_{ij})(r_{i+1,j}-r_{ij}) \end{bmatrix}$$

$$+ p_{i-1,j-1} \begin{bmatrix} (r_{ij}+r_{i,j-1}+r_{i-1,j})(z_{i-1,j}-z_{i,j-1}) \\ + (z_{i,j-1}-z_{ij})(r_{i-1,j}-r_{ij}) \\ - (z_{i-1,j}-z_{ij})(r_{i,j-1}-r_{ij}) \end{bmatrix}$$

$$\frac{3}{\pi} M_{ij} \frac{(z_{ij}^{t+\Delta t} - 2z_{ij}^{t} + z_{ij}^{t-\Delta t})}{\Delta t^2} = p_{i-1,j} \left[r_{ij}+r_{i-1,j}+r_{i,j+1}\right]\left[r_{i-1,j}-r_{i,j+1}\right]$$

$$+ p_{ij} \left[r_{ij}+r_{i,j+1}+r_{i+1,j}\right]\left[r_{i,j+1}-r_{i+1,j}\right]$$

$$+ p_{i,j-1} \left[r_{ij}+r_{i+1,j}+r_{i,j-1}\right]\left[r_{i+1,j}-r_{i,j-1}\right]$$

$$+ p_{i-1,j-1} \left[r_{ij}+r_{i,j-1}+r_{i-1,j}\right]\left[r_{i,j-1}-r_{i-1,j}\right].$$